Colloqui della Classe di Scienze

Anno Accademico 2015/2016

Sala Azzurra | Palazzo della Carovana
Scuola Normale Superiore
Piazza dei Cavalieri, 7 - PISA

11 MAGGIO 2016
ore 15.00

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New approaches in electronic structure theory: The density matrix renormalization group

Abstract

In electronic structure theory, the density matrix renormalization group (DMRG) algorithm has become a competitive multi-configuration self-consistent field (MCSCF) method that allows us to access large active orbital spaces beyond the capabilities of traditional complete active space self-consistent field (CASSCF) approaches. An advantage of DMRG is the iterative nature of the algorithm. While this could be viewed as a drawback (many iterations are needed and convergence can feature plateaus with little change in energy), the qualitative nature of the DMRG wave function is well reproduced already after comparatively few iterations. This knowledge can be exploited for solving the active-space selection problem in MCSCF approaches. Recently, we have shown that concepts from quantum information theory can be used to classify active orbital spaces so that they can be constructed from partially converged DMRG calculations.

Elaborazione a cura del Servizio Comunicazione e Relazioni Esterne | SNS

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